



# Leadership Computing Facility Oak Ridge Users Meeting

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# 2006 DOE Strategic Plan

## Advanced Scientific Computing Research Program

### Strategic Theme 3: Scientific Discovery and Innovation



- **Goal 3.1: Scientific Breakthroughs** – Achieve the major scientific discoveries that will drive U. S. competitiveness, inspire America, and revolutionize approaches to the Nation's energy, national security, and environmental quality challenges.
  - Strategy: Advance the computational sciences and the leadership-class computational capabilities required for today's frontiers of scientific discovery.
- **Goal 3.2: Foundations of Science** – Deliver the scientific facilities, train the next generation of scientists and engineers, and provide the laboratory capabilities and infrastructure required for U.S scientific primacy.
  - Strategy:
    - Complete construction and begin operation of major scientific user facilities
    - Better communicate the importance of science and technology to inspire participation in the innovation economy
- **Goal 3.3: Research Integration** – Integrate basic and applied research to accelerate innovation and to create transformational solutions for energy and other U. S. needs.
  - Strategy: Strengthen ties between the basic research and applied mission programs in Departmental planning.

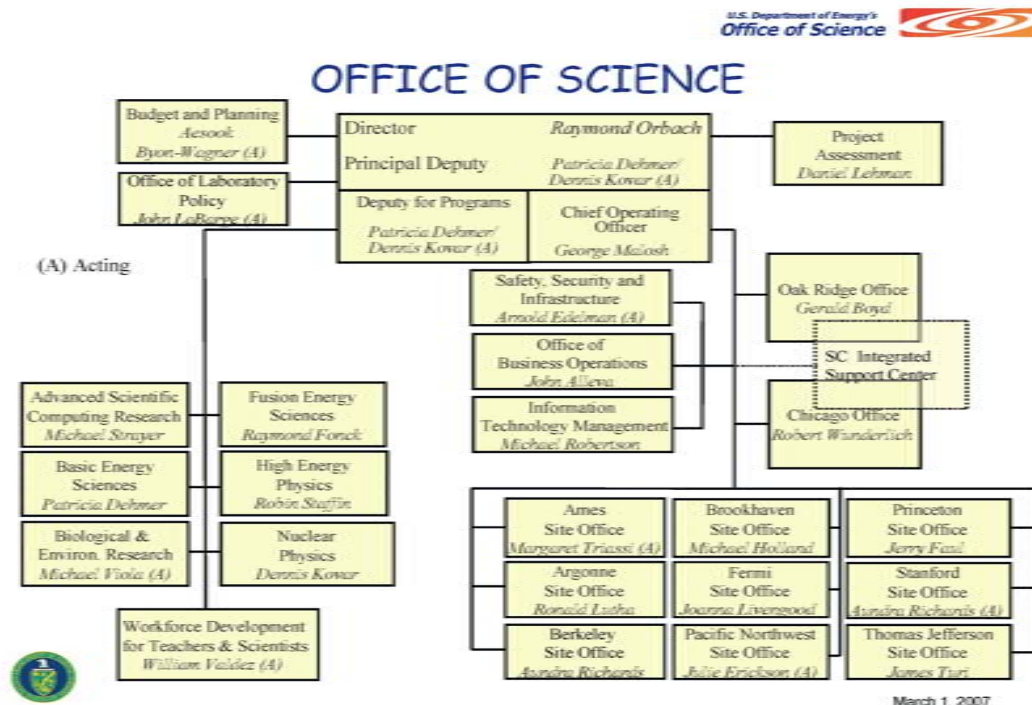
(<http://www.energy.gov/about/strategicplan.htm> )



Office of Science

# Office of Science Organization

Advanced Scientific Computing Research Program





# Road to the Petascale

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## Advanced Scientific Computing Research Program

### In the President's State of the Union Address on **January 31, 2006**

***"I propose to double the federal commitment to the most critical basic research program in the physical sciences over the next ten years. This funding will support the work of America's most creative minds as they explore promising areas such as nanotechnology, [supercomputing](#), and alternative energy sources."***

### In the President's State of the Union Address on **January 23, 2007**

***"It's in our vital interest to diversify America's energy supply – [the way forward is through technology...](#)"***



Office of Science

# FY2008 Budget Request Advanced Scientific Computing Research (ASCR)

## Advanced Scientific Computing Research Program

(dollars in thousands)

FY 2006 Current Appropriation	FY 2007 Request	FY 2007 House Mark	FY 2007 Senate Mark	FY 2007 Appropriation	FY 2008 Request
228,382 <sup>[a]</sup>	318,654	318,654	318,654	***	340,198

FY 2008 President's Budget Request for ASCR includes

- \$130M for Applied Mathematics, Computer Science and Computational Partnerships Research;
- \$201M for High Performance Computing and Network Facilities and Testbeds
  - **Includes \$77M for Leadership Computing at Oak Ridge to acquire 1 petaflop Cray Baker System**
- \$9M for Small Business Innovative Research

<sup>[a]</sup> Total is reduced by \$2,371,000 for a rescission in accordance with P.L. 109-148, the Emergency Supplemental Act to Address Hurricanes in the Gulf of Mexico and Pandemic Influenza, 2006; \$5,627,000, which was transferred to the SBIR program; and \$675,000, which was transferred to the STTR program.



# Innovative and Novel Computational Impact on Theory and Experiment- INCITE

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## Advanced Scientific Computing Research Program

- Initiated in 2004
- Provides Office of Science computing resources to a small number of computationally intensive research projects of large scale, that can make high-impact scientific advances through the use of a large allocation of computer time and data storage
- Open to national and international researchers, including industry
- No requirement of DOE Office of Science funding
- Peer-reviewed
- 2004 Awards: 4.9 Million processor hours at NERSC awarded to three projects
- 2005 Awards: 6.5 Million processor hours at NERSC awarded to three projects



# INCITE 2006

## Advanced Scientific Computing Research Program

Wired Magazine, August, 2006, pg. 42



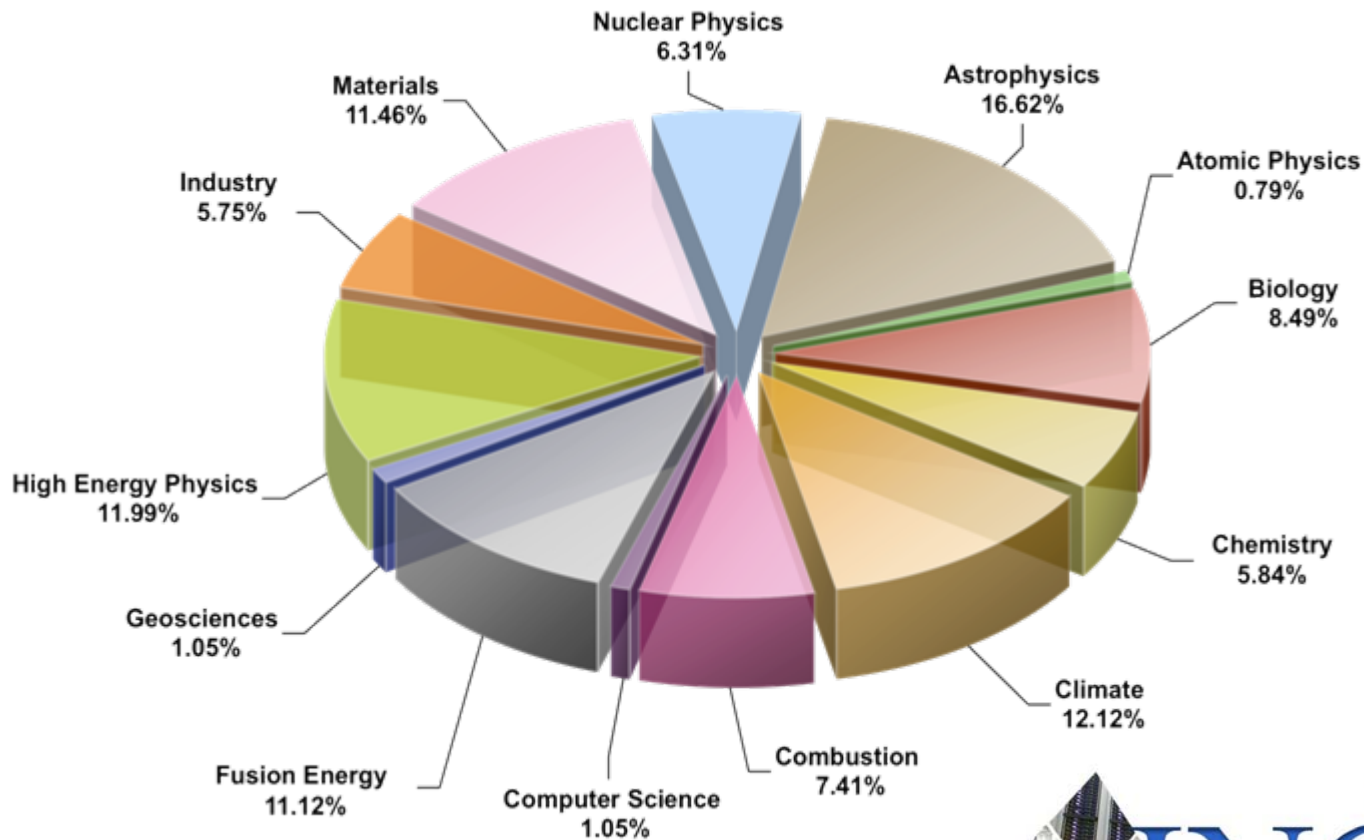
- Expanded to include SC high end computing resources at PNNL, ORNL and ANL in addition to LBNL and multiple year requests.
- Received 43 proposals requesting over 95 million processor hours.
  - 60% from Universities
  - 40% had funding from other federal research agencies
- 15 Awards for over 18.2 million processor hours





# 2007 INCITE Allocations by Disciplines

## Advanced Scientific Computing Research Program



95 Million  
processor hours  
allocate to 45  
projects

80% of resources  
at LCF allocated  
through INCITE

<http://www.science.doe.gov/ascr/incite>



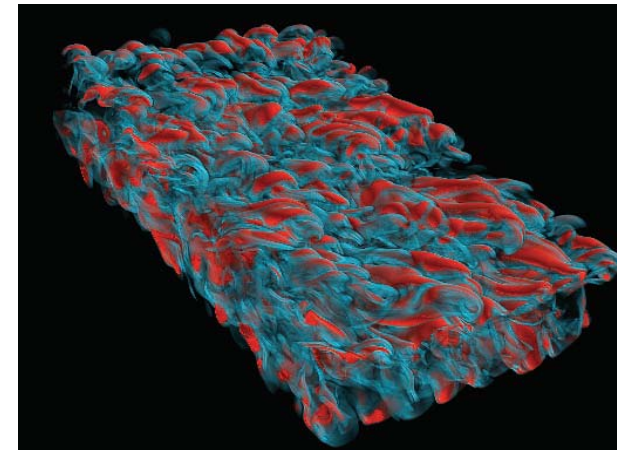




# INCITE Accomplishments

## Advanced Scientific Computing Research Program

- “The INCITE award has enabled us to extend our computations to three dimensions so that we may investigate interactions between turbulence, mixing, and finite-rate detailed chemistry in combustion.”  
**Direct Numerical Simulation of Turbulent Non-Premixed Combustion (Jacqueline Chen, Sandia National Laboratories, California)**
- “Using our 2006 INCITE award, we have simulated fracture of the largest-ever 3-D lattice systems. For the first time, these simulations confirmed and explained the anomalous scaling observed in fracture experiments, a result which could only be achieved by simulating very large systems. These large scale simulations, possible only through INCITE allocation, have been instrumental in advancing the current understanding of physics of how materials fracture.”  
**Large Scale Simulations of Fracture in Disordered Media: Statistical Physics of Fracture, Phani Nukala, Oak Ridge National Laboratory, Tennessee**



**NERSC – INCITE - Chen**

*Simulated planar jet flame, colored by the rate of molecular mixing, critical for determining the interaction between reaction and diffusion in a flame.*

See <http://www.sc.doe.gov/ascr/incite/ResearcherRemarks.pdf>



# 2007 INCITE Accomplishment

## Advanced Scientific Computing Research Program

The screenshot shows the DOE Science ASCR homepage. The browser window title is "DOE - Science - ASCR - Homepage - Mozilla Firefox". The address bar shows "http://www.science.doe.gov/ascr/". The page features the U.S. Department of Energy logo and the Office of Science logo. A navigation bar includes links for HOME, ORGANIZATION, NEWS, CONTACT US, and a SEARCH box. Below the navigation bar, there are sections for "What is Scientific Computing?", ASCAC, FACILITIES, RESEARCH, and SBIR/STTR. The main content area is titled "ASCR The Office of Advanced Scientific Computing Research". It features a headline "DOE Supercomputers Used by Scientists to Compute Death Throes of White Dwarf Star in 3D Simulations" with a 3D simulation image. The text describes how University of Chicago scientists demonstrated the detonation of a white dwarf star in a more realistic three-dimensional simulation using supercomputers operated by the U.S. Department of Energy (DOE). The simulation confirmed what the team already suspected from previous tests: that the stars detonate in a supersonic process resembling diesel-engine combustion. A "more..." link is provided. Below this, a section titled "DOE's Office of Science Awards 95 Million Hours of Supercomputing Time to Advance Research in Science, Academia and Industry" reports that the U.S. Department of Energy's (DOE) Office of Science announced today that 45 projects were awarded a total of 95 million hours of computing time on some of the world's most powerful supercomputers as part of its 2007 INCITE program. DOE's Under Secretary for Science Dr. Raymond Orbach presented the awards at the Council on Competitiveness in Washington, DC. A "more..." link and a "View the Event Video..." link are provided. The "MISSION" section states that the mission of the Advanced Scientific Computing Research (ASCR) program is to deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy. In the past two decades, leadership in scientific computation has become a cornerstone of the Department's strategy to ensure the security of the nation. The right sidebar includes a "WHAT'S NEW IN ASCR" section with a "Monthly News Roundup" and a "SciDAC Review Volume 3" link. Below this is a "Related Links of Interest" section with logos for the U.S. Department of Energy, Office of Science, SBIR, INCITE, Advanced Simulation & Computing, SciDAC, and National Leadership.



# 2009 INCITE Accomplishment

Advanced Scientific Computing Research Program

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